

## Connecting via Winsock to STN

STN Structure 01/16/2008  
Search ( Registry / CapIns )  
Cmpd Claims 20, 23, 32, 36, 41

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LOGINID:SSPTAJMN1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS 1	Web Page for STN Seminar Schedule - N. America	
NEWS 2	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 3	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 4	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 5	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 6	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 7	AUG 27	USPATOLD now available on STN
NEWS 8	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 9	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 10	SEP 13	FORIS renamed to SOFIS.
NEWS 11	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS 12	SEP 17	CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 13	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS 14	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 15	OCT 02	CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 16	OCT 19	BEILSTEIN updated with new compounds
NEWS 17	NOV 15	Derwent Indian patent publication number format enhanced
NEWS 18	NOV 19	WPIX enhanced with XML display format
NEWS 19	NOV 30	ICSD reloaded with enhancements
NEWS 20	DEC 04	LINPADOCDB now available on STN
NEWS 21	DEC 14	BEILSTEIN pricing structure to change
NEWS 22	DEC 17	USPATOLD added to additional database clusters
NEWS 23	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS 24	DEC 17	DGENE now includes more than 10 million sequences
NEWS 25	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS 26	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 27	DEC 17	CA/CAplus enhanced with new custom IPC display formats
NEWS 28	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS 29	JAN 02	STN pricing information for 2008 now available
NEWS EXPRESS	19 SEPTEMBER 2007:	CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

10/539, 151

01/16/2008

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NEWS IPC8      For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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STRUCTURE FILE UPDATES: 15 JAN 2008 HIGHEST RN 1000000-66-7  
DICTIONARY FILE UPDATES: 15 JAN 2008 HIGHEST RN 1000000-66-7

New CAS Information Use Policies, enter HELP USAGE TERMS for details.

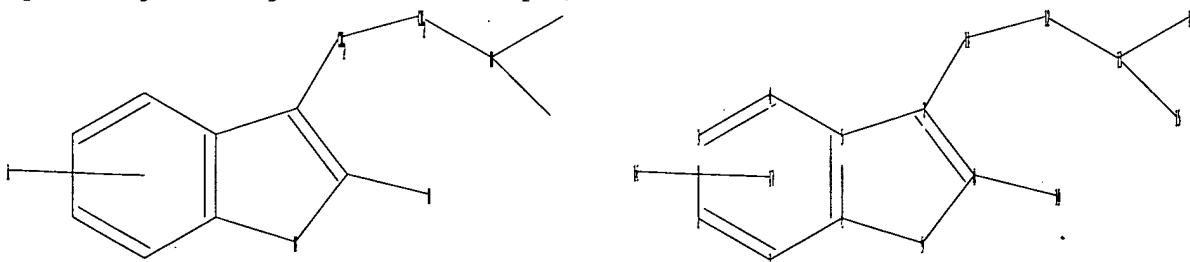
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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=> Uploading C:\Program Files\Stnexp\Queries\10539151\Jan1.str
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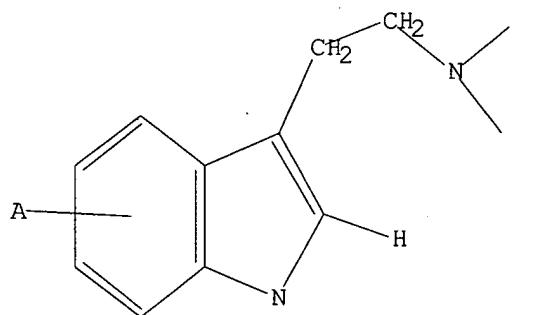
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 13-14 13-15  
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Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom

L1 STRUCTURE UPLOADED

=> d  
 L1 HAS NO ANSWERS  
 L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11  
 SAMPLE SEARCH INITIATED 11:29:53 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 17947 TO ITERATE

11.1% PROCESSED 2000 ITERATIONS 40 ANSWERS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 350918 TO 366962  
 PROJECTED ANSWERS: 6042 TO 8314

10/539,151

01/16/2008

=> s 11 full ✓  
FULL SEARCH INITIATED 11:30:14 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 356284 TO ITERATE

100.0% PROCESSED ✓ 356284 ITERATIONS  
SEARCH TIME: 00.00.02

L3 5875 SEA SSS FUL L1

=> fil caplus  
COST IN U.S. DOLLARS  
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
178.36	178.57

FILE 'CAPLUS' ENTERED AT 11:30:27 ON 16 JAN 2008  
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FILE COVERS 1907 - 16 Jan 2008 VOL 148 ISS 3  
FILE LAST UPDATED: 15 Jan 2008 (20080115/ED)

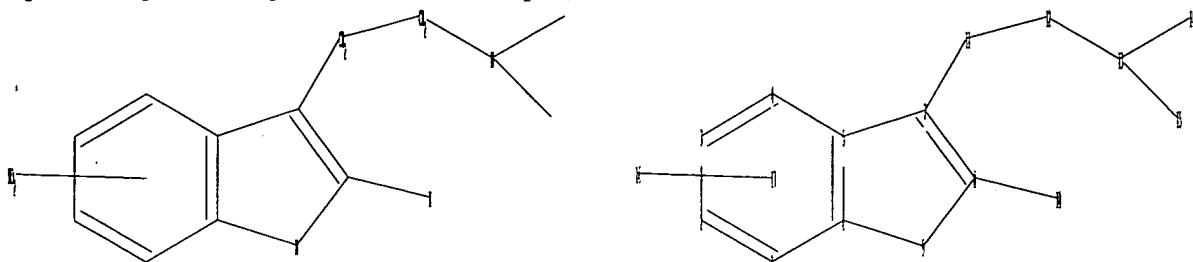
Effective October 17, 2005, revised CAS Information Use Policies apply.  
They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 13  
L4 4163 L3  
=> d ibib abs hitstr 4163

5875 ANSWERS

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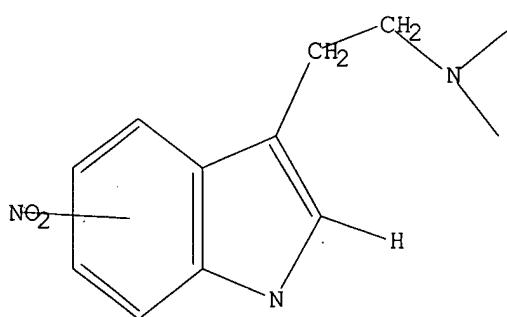


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ring nodes :  
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ring/chain nodes :  
13 14 15  
chain bonds :  
7-11 8-10 11-12 12-13  
ring/chain bonds :  
13-14 13-15  
ring bonds :  
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exact/norm bonds :  
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exact bonds :  
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normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom

L5 STRUCTURE UPLOADED

=> d  
L5 HAS NO ANSWERS  
L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15 full sub=13

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 11:32:51 FILE 'REGISTRY'  
FULL SUBSET SCREEN SEARCH COMPLETED - 246 TO ITERATE

100.0% PROCESSED 246 ITERATIONS  
SEARCH TIME: 00.00.01

37 ANSWERS

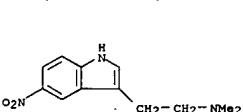
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SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH  
L7 22 L6

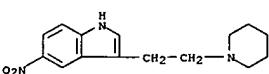
=> d ibib abs hitstr 22

L7 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
 ACCESSION NUMBER: 1954:25005 CAPLUS  
 DOCUMENT NUMBER: 48:25005  
 ORIGINAL REFERENCE NO.: 48:4512a-1,4513a-e  
 TITLE: The synthesis of nitro- and aminoindoles analogous to serotonin  
 AUTHOR(S): Shaw, Elliott; Woolley, D. W.  
 CORPORATE SOURCE: Rockefeller Inst. for Med. Research, New York, NY  
 SOURCE: Journal of the American Chemical Society (1953), 75, 1877-81  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 48:25005  
 GI For diagram(s), see printed CA Issue.  
 AB A series of new 3-alkyl- and 2,3-dialkylnitroindoles has been prepared by the Fischer rearrangement. Aldehyde *p*-nitrophenylhydrazones have been converted with concentrated HCl in a biphasic system at room temperature to 3-alkyl-5-nitroindoles for the first time. A number of aminoindoles was readily prepared from the corresponding nitroindoles by reduction with Na2S2O4; other reducing agents led to mixts. The appropriate ketone *p*-nitrophenylhydrazones refluxed 3 h. with concentrated HCl (10 cc./g.) gave the corresponding indoles which were filtered off and washed with concentrated HCl and then with H2O. In this manner were prepared the following substituted 5-nitroindoles (substituents, % yield, and m.p. given): 2-Me, 3-Bu, 21, 125-6° (from C6H6-hexane); and 2-Me, 3-Cl(CH2)2, 32, 204-5° (from C6H6). The 2,3,3-tri-Me derivative, m. 124-5°, prepared in 48% yield by this method from *p*-O2NC6H4NNH:CHMe2 remained in solution and was precipitated by neutralizing the mixture. Crude 2-methyl-3-ethyl-5-nitroindole, prepared similarly, was purified by dissolving in boiling C6H6 (20 cc./g.), filtering, treating the filtrate near the b.p. with Al2O3 (1.5 g./l. g. crude base), evaporating the solution to 0.2 volume, and recrystall. the solid from EtOH to give the pure product, m. 190-1°. *p*-O2NC6H4NNH:CHPr (10 g.) was dissolved in a suspension of 5 g. *p*-O2NC6H4NNH2 in 200 cc. concentrated HCl, a 200-mL layer of C6H6 added, the mixture stirred 3 h., the C6H6 replaced by fresh solvent, the mixture stirred again 3 h., the combined C6H6 layers were washed with H2O, dried with MgSO4, concentrated to about 25 cc., and the solution chromatographed on Al2O3 with C6H6 to yield 2.2 g. 3-ethyl-5-nitroindole, m. 94-5° (from C6H6-hexane), and, eluted with EtOH, 1.1 g. crystalline solid, m. 237-8°, apparently 1,1-bis(3-ethyl-5-nitro-2-indolyl)butane. The Et2O extract from a HIO4 cleavage of 245 g. isomeric chloropentanediols (cf. Paul and Tchelitcheff, C.A. 42, 4944f) was concentrated in vacuo 1 h., and the residue added to 100 g.

L7 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
 (inflection) (2.8), 408-12 (4.35), min. 295 (1.1); 5-NO2 isomer of IX, max. 276-7 (21.0), 336-7 (9.25), min. 240 (5.65), 305 (4.5); 6-NO2 isomer, max. 251 (9.1), 272 (6.2) 340-50 (7.1), 395-400 (9.25), min. 265 (5.9), 295 (2.3); 7-NO2 isomer, max. 240 (10.6), 259-60 (10.2), 372-8 (6.28), min. 250 (9.25), 300 (0.5); VI, max. 230 (31.0), 277-9 (6.8), min. 253 (3.6), 288-93 (6.05); max. 284-6 (6.84), 231-2 (24.7), min. 260 (3.74); VII, max. 235 (30.9), 273-5 (5.5), 307 (5.1), min. 255 (4.0), 290 (3.25); and VIII, max. 228 (35.8), 275-7 (8.5), 300 (inflection) (4.5), min. 250 (3.8). 2,3-Dimethyl-5-aminindole (0.5 g.) and 0.32 g. OC(CH2)2CO.0 heated 2 min. in an oil bath at 125°, the melt taken up in aq. Na2CO3, and the soln. gradually acidified gave 0.62 g. 2,3-dimethyl-5-succinimidindole, m. 147-8°; the mixt. heated longer gave 2,3-dimethyl-5-succinimidindole, m. 198-9°, insol. in aq. Na2CO3.  
 IT 2957956-33-7P, Indole, 3-(2-dimethylaminoethyl)-5-nitro-, hydrochloride 858828-08-7P, Piperidine, 1-[2-(5-nitro-3-indolyl)ethyl]- 860198-58-9P, Indole, 5-nitro-3-(2-octahydro-1-(2H)-quinolyl)ethyl-, hydrochloride 860359-59-7P, Indole, 5-nitro-3-(2-piperidinoethyl)-, hydrochloride  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 2957956-33-7 CAPLUS  
 CN 1H-Indole-3-ethanamine, N,N-dimethyl-5-nitro-, monohydrochloride (9CI) (CA INDEX NAME)



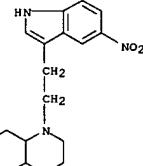
RN 858828-08-7 CAPLUS  
 CN Piperidine, 1-[2-(5-nitro-3-indolyl)ethyl]- (9CI) (CA INDEX NAME)



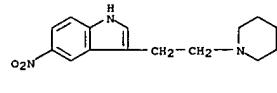
RN 860198-58-9 CAPLUS  
 CN Quinoline, decahydro-1-[2-(5-nitro-3-indolyl)ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

L7 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
 p-O2NC6H4NNH2 in 2 l. 50% AcOH to give 103 g. p-O2NC6H4NNH:CH(CH2)2CH2Cl (1), m. 101-2°. I (15 g.) stirred with two 750-cc. portions of C6H6 as described before, and the product resolved on Al2O3 gave 2.0 g. (15%) 3-(2-chloroethyl)-5-nitroindole (II), m. 120-1°; 5% 3-(2-hydroxyethyl)-5-nitroindole, m. 97-8°; 0.5 g. unidentified crystals, m. 134-5° (from C6H6-hexane); and 1.63 g. unidentified material, m. 82-3° (from aq. EtOH). II (1 g.) in 75 cc. EtOH let stand 10 days at room temp. with 50 cc. concd. NH4OH, the EtOH removed, the residual aq. suspension acidified with 6N HCl, filtered hot, and the filtrate treated slowly with alkali gave 0.63 g. (6%) 5-nitrotryptamine, m. 136-9°. II (1 g.) in 60 cc. EtOH let stand 4 days at room temp. with 40 cc. aq. 25% Me2NH, the EtOH removed in vacuo, and the pptd. base washed with H2O and treated with 6N HCl gave 57% 3-(2-dimethylaminoethyl)-5-nitroindole-HCl, m. 268-70° (from 95% EtOH). Similarly were prep'd. the following analogous 3-substituted 5-nitroindole-HCl (substituent, % yield, and m.p. given): 2-piperidinoethyl, 51, 272-3° (from 95% EtOH); 2-(decahydro-1-quinolyl)ethyl, 10, 254-6° (from 95% EtOH); and 2-[(2-(4-imidazolyl)ethyl)aminoethyl, dipicrate, 24%, 207-8° (from aq. Me2CO). 2-Methyl-3-(2-chloroethyl)-5-nitroindole (1.5 g.) in 75 cc. EtOH gave similarly with 30 cc. concd. NH4OH 75% 2-methyl-5-nitrotryptamine-HCl, m. 265-6°. In the same manner was obtained 88% 2-methyl-3-(2-piperidinoethyl)-5-nitroindole-HCl, m. 275-7° (from 95% EtOH). 2,3-Dimethyl-5-nitroindole (III), (3.8 g.) in 300 cc. PhMe distd. with 20 cc. m. alc. EtONa until the b.p. of PhMe was reached, the residue refluxed, treated with excess MeI, filtered, the filtrate evapd. to dryness, and the residue chromatographed on Al2O3 with C6H6 gave 2.1 g. (51%) 1,2,3-trimethyl-5-nitroindole, m. 136-9° (from C6H6-hexane). III (0.85 g.) oxidized with 0.85 g. CrO3 in glacial AcOH and the crude oxidn. product hydrolyzed with aq. alc. HCl gave 0.22 g. ketone, m. 148-50° (from aq. EtOH). III (5 g.) in 175 cc. EtOH and 100 cc. N NaOH treated at 50° with 25 g. Na2S2O4 in 120 cc. 0.5N NaOH, the almost colorless soln. filtered hot, the inorg. residue washed with EtOH, the alc. filtrate and washing concd. in vacuo, and the solid filtered off and recrystall. from EtOH gave 2.2 g. (52%) 2,3-dimethyl-5-aminindole, m. 173-4° (from aq. EtOH). Similarly were prep'd. the following aminoindoles (substituent, % yield, and m.p. given): 3-ethyl-5-amino (IV), 45, 116-18°; 2-Me deriv. (V), 64, 148-9°; 2,3-dimethyl-5-amino, 64, 96-8°; 2,3-dimethyl-4-amino (VI), 50, 156-60°; 2,3-dimethyl-6-amino (VII), 50, 117-18°; 2-methyl-3-ethyl-7-amino (VIII), 40, 110-12°; 1,2,3-trimethyl-5-amino, picrate, 41, 203-5° (from aq. EtOH); 3-(2-dimethylaminoethyl)-5-amino, dipicrate, 38, 202-4° (from H2O); 3-(2-piperidinoethyl)-5-amino, dipicrate, 67, 211-12° (from aq. EtOH); 2-methyl-3-(2-piperidinoethyl)-5-amino, 45, 149-51°; 5-aminotryptamine dipicrate, 60, 204-5° (from H2O); 2-methyl-5-aminotryptamine 40, 112°; and 6-amino-1,2,3,4-tetrahydrocarbazole, 64, 146-7°. The UV absorption max. and min. in mu are, in parentheses, the corresponding c + 10-3 values are for: 2-methyl-3-ethyl-4-nitroindole (IX), max. 240-5 (8.6), 340

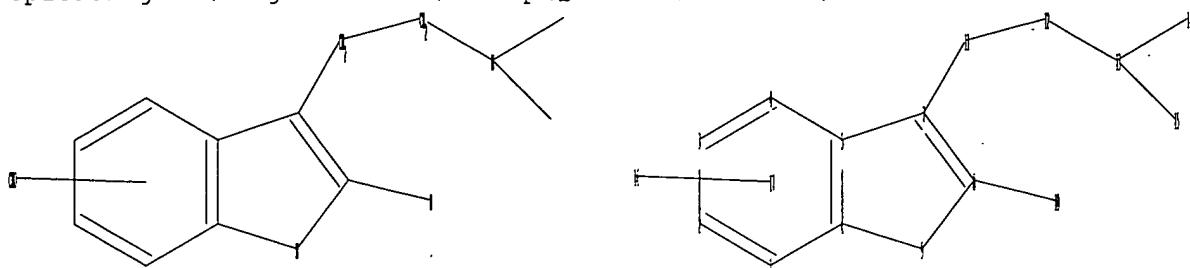
L7 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 860359-59-7 CAPLUS  
 CN Indole, 5-nitro-3-(2-piperidinoethyl)-, hydrochloride (9CI) (CA INDEX NAME)



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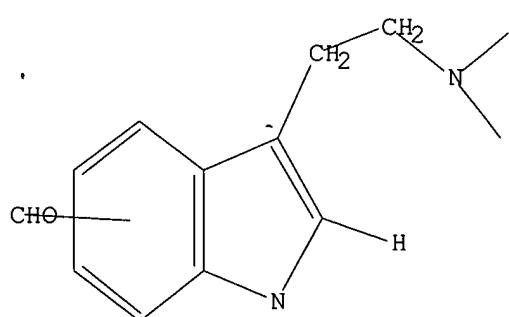


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Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom

L8 STRUCTURE UPLOADED

=> d  
L8 HAS NO ANSWERS  
L8 STR



claim 32

10/539,151

01/16/2008

Structure attributes must be viewed using STN Express query preparation.

=> s 18 full sub=13

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 11:34:12 FILE 'REGISTRY'  
FULL SUBSET SCREEN SEARCH COMPLETED - 5875 TO ITERATE

100.0% PROCESSED 5875 ITERATIONS  
SEARCH TIME: 00.00.01

10 ANSWERS

L9 10 SEA SUB=L3 SSS FUL L8

SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH  
L10 8 L9

=> d ibib abs hitstr 8

L10 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:626347 CAPLUS

DOCUMENT NUMBER: 105:226347

ORIGINAL REFERENCE NO.: 105:36543a,36546a

TITLE: Indole derivatives and pharmaceutical compositions containing them

INVENTOR(S): Bays, David Edmund; Webb, Colin Frederick

PATENT ASSIGNEE(S): Glaxo Group Ltd. UK

SOURCE: Ger. Offen., 60 pp.

CODEN: GWXK BX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

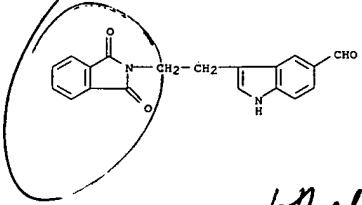
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3543982	A1	19860619	DE 1985-3543982	19851212
BE 903846	A1	19860612	BE 1985-216004	19851212
SE 8505887	A	19860614	SE 1985-5887	19851212
GB 2168347	A	19860618	GB 1985-30591	19851212
GB 2168347	B	19880203		
AU 8551151	A	19860619	AU 1985-51151	19851212
AU 579687	B2	19881201		
FR 2574793	A1	19860620	FR 1985-18416	19851212
FR 2574793	B1	19881014		
NL 8503424	A	19860701	NL 1985-3424	19851212
JP 61151172	A	19860709	JP 1985-278124	19851212
ZA 8509520	A	19860827	ZA 1985-9520	19851212
CH 667454	A5	19881014	CH 1985-5301	19851212
PRIORITY APPLN. INFO.:			GB 1984-31426	A 19841213

OTHER SOURCE(S): CASREACT 105:226347; MARPAT 105:226347  
GI

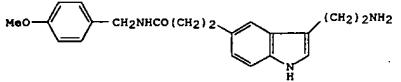
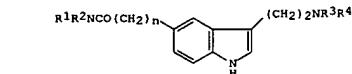
L10 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
 R3, R4 = H, Cl-3 alkyl, 2-propenyl; n = 2-5) and their physiol. tolerable salts and solvates, useful as selective vasoconstrictors for cranial vessels at 0.5-50 mg, were prep'd. by 7 methods. 4-H2NC6H4(CH2)2CO2H was diazotized and the product reduced with SnCl2 to give 4-H2NNC6H4(CH2)2CO2H.HCl, which reacted with 2-(4,4-diepoxybutyl)-1H-isoindole-1,3(2H)-dione in refluxing eq. AcOH to give 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]-1H-indole-5-propanoic acid. Successive reaction with pivaloyl chloride and 4-MeOCH2CH2NH2 gave the N-(4-methoxyphenyl)methylpropanamide analog, hydrolysis of which gave indolylethylamine II, characterized as the hemisuccinate. Formulations for tablets, capsules, suppositories, and i.v. injection solns. were given.

IT 105323-64-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (Preparation and Wittig reaction of)

RN 105323-64-6 CAPLUS  
 CN 1H-Indole-5-carboxaldehyde, 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]- (CA INDEX NAME)



pthal - proviso



AB Indoles I [R1 = H, Cl-6 alkyl, C3-7 cycloalkyl, C3-6 alkenyl, Ph or phenyl-Cl-4-alkyl with Ph (un)substituted by Cl-3 alkoxy, OH, halo, R5R6NCO (R5, R6 = H, Cl-3 alkyl), R7R8N (R7, R8 = H, Cl-3 alkyl; R7R8N = saturated monocyclic 5-7 membered ring); R2 = H, Cl-6 alkyl; R1R2N = R7R8N;

L10 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:575786 CAPLUS

DOCUMENT NUMBER: 107:175786

TITLE: Preparation of 5-(2-aminoethyl)tryptamines as antimigraine agents

INVENTOR(S): Mills, Keith; Coates, Ian Harold; Bays, David Edmund; Webb, Colin Frederick; Dowle, Michael Dennis

PATENT ASSIGNEE(S): Glaxo Group Ltd., UK

SOURCE: Ger. Offen., 17 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

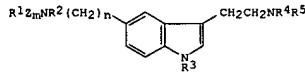
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3700407	A1	19870709	DE 1987-3700407	19870108
AU 8767418	A	19870709	AU 1987-67418	19870108
AU 597324	B2	19900531		
NL 8700027	A	19870803	NL 1987-27	19870108
GB 2186874	A	19870826	GB 1987-381	19870108
GB 2186874	B	19900207		
FR 2595352	A1	19870911	FR 1987-108	19870108
FR 2595352	B1	19900713		
JP 62228057	A	19871006	JP 1987-2590	19870108
AT 8700024	A	19871215	AT 1987-24	19870108
AT 386197	B	19880711		
ZA 8700104	A	19871230	ZA 1987-104	19870108
BE 1000072	A1	19880202	BE 1987-4	19870108
CH 671017	A5	19890731	CH 1987-46	19870108
			GB 1986-398	A 19860108

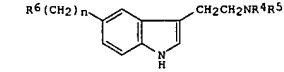
PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 107:175786

GI



I



II

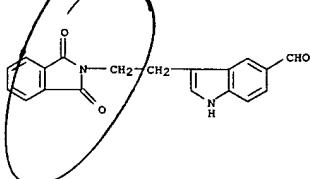
AB The title compds. (I: R1 = H, C1-6 alkyl, C3-7 cycloalkyl, Ph, phenyl-C1-4 alkyl; R2, R3 = H, C1-3 alkyl; R4, R5 = CH2CH:CH2, R3; Z = CO, SO2; n = 2-5; m = 1) were prepared as antimigraine agents (no data). 4-H2NNHC6H4CH2CN was refluxed with 4-phthalimidobutanal di-Et acetal in

L10 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
H2O/HOAc to give tryptamine II (NR4R5 = phthalimido, R6 = cyano, n = 1) which, on hydrogenation over PdO/C, gave II.HCl (NR4R5 = phthalimido, R6

NH2, n = 2). This was stirred with Ac2O in pyridine and the product refluxed with H2NNH2 in EtOH to give II (R4 = R5 = H, R6 = AcNH, n = 2). Tablets were prepd. each contg. II (R4 = R5 = Me, R6 = 4-AcNHG6H4CH2CONH, n = 2) 2.4, CaHPO4 95.1, Croscarmellose Na 2.0, and Mg stearate 0.5 mg. 105323-64-6P

IT R1: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and Wittig reaction of)

RN 105323-64-6 CAPLUS  
CN 1H-Indole-5-carboxaldehyde, 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl] (CA INDEX NAME)



X



L10 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:245114 CAPLUS

DOCUMENT NUMBER: 120:245114

TITLE: Preparation of heteroaromatic 5-hydroxytryptamine receptor agonists

INVENTOR(S): Castro Pineiro, Jose Luis; Matessa, Victor Giulio

PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK

SOURCE: PCT Int. Appl., 43 pp.

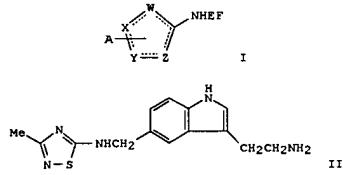
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9321182	A1	19931028	WO 1993-GB789	19930414
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9340766	A	19931118	AU 1993-40766	19930414
EP 636131	A1	19950201	EP 1993-910152	19930414
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07505649	T	19950622	JP 1993-518132	19930414
US 5510359	A	19960423	US 1994-318610	19941007
PRIORITY APPLN. INFO.:			GB 1992-8463	A 19920416
			WO 1993-GB789	A 19930414

OTHER SOURCE(S): MARPAT 120:245114  
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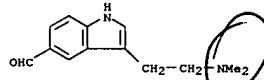
AB Title compds. I (W, X, Y, Z = O, S, N, C such that one of W, X, Y, Z = O, S and at least one of W, X, Y, Z = C; A = H, hydrocarbyl, heterocycl, halo, NC, F3C, RXO, RXs, RYRXN, RYCORXN, RyO2CRXN, etc. wherein RX, Ry = H, hydrocarbyl, heterocycl, RXRY = C2-6 alkylene; E = bond, C13-4 alkylene; F = substituted heterocycl) or a salt thereof, are prepared

To 5-(aminomethyl)-3-[2-(N-tert-butoxycarbonylamino)ethyl]-14-indole (preparation given) in THF and (Me2CH)2NET was added 5-chloro-3-methyl-1,2,4-

L10 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
thiadiazole to give the protected thiadiazolylamine which in CH2Cl2 was reacted with F3CCO2H to give the title compd. II. The activity of I as agonists of 5-HT1 receptors was measured as to their ability to mediate contraction of the saphenous vein and calcd. as -log10EC50(pEC50) from plots of % 5-HT (1  $\mu$ M) response against the concn. of the agonist and was not less than 5.0. A tablet formulation comprising I is given.

IT 152673-51-3P 152673-52-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

RN 152673-51-3 CAPLUS  
CN 1H-Indole-1-carboxylic acid, 3-(2-(dimethylamino)ethyl)-5-formyl-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 152673-52-4 CAPLUS  
CN 1H-Indole-1-carboxylic acid, 3-(2-(dimethylamino)ethyl)-5-formyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

L10 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:152309 CAPLUS

DOCUMENT NUMBER: 134:193415

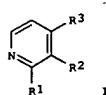
TITLE: Preparation of heteroannelated pyridines as 5-HT1A receptor ligands  
INVENTOR(S): Peglion, Jean-louis; Dessinges, Aimee; Poitevin, Christophe; Milan, Mark; Dekeyne, Anne  
PATENT ASSIGNEE(S): Adir Et Compagnie, Fr.; Les Laboratoires Servier  
SOURCE: Eur. Pat. Appl., 27 pp.DOCUMENT TYPE: Patent  
LANGUAGE: French  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1078928	A1	20010228	EP 2000-402359	20000825
EP 1078928	B1	20040512		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
FR 2797874	A1	20010302	FR 1999-10834	19990827
FR 2797874	B1	20020329		
US 6399616	B1	20020604	US 2000-641777	20000818
JP 2001057978	A	20010410	JP 2000-252191	20000823
JP 3602780	B2	20041215		
MX 2000PA08241	A	20020820	MX 2000-PA8241	20000823
CA 2317053	A1	20010227	CA 2000-2317053	20000825
ZA 2000004411	A	20010228	ZA 2000-4411	20000825
CN 1286255	A	20010307	CN 2000-124065	20000825
HU 2000003413	A2	20010730	HU 2000-3413	20000825
HU 2000003413	A3	20031128		
AT 266664	T	20040515	AT 2000-402359	20000825
PT 1078928	T	20040930	PT 2000-402359	20000825
ES 220359	T3	20041216	ES 2000-402359	20000825
NO 2000004295	A	20010228	NO 2000-4295	20000828
NO 316651	B1	20040322		
BR 2000003848	A	20010403	BR 2000-3848	20000828
AU 765661	B2	20030925	AU 2000-53642	20000828
HK 1034250	A1	20050429	HK 2001-104815	20010711
US 2002161228	A1	20021031	US 2002-105171	20020325
US 6486171	B2	20021126		
PRIORITY APPLN. INFO.: FR 1999-10834 A 19990827				
US 2000-641777 A3 20000818				

OTHER SOURCE(S): MARPAT 134:193415  
GI

L10 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

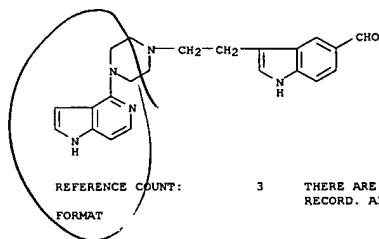
(Continued)



AB Title compds. {I; R1 = R(CH2)nZZ1; R = (un)substituted naphthyl or heteroannelated Ph; R2R3 = atoms to complete a thiophene, furan, or (oxol)pyrrole ring; Z = bns, O, [(ar)alkyl]imino; ZZ1 = 1,4-cyclohexylene, piperidine-1,4- or -4,1-diyl, piperazine-1,4-diyl; n = 1-6} were prepared. Thus, 7-chlorofuro[2,3-c]pyridine was aminated by N-(2-naphthylmethyl)-4-piperidinemamine to give I (R1 = RCH2NHZ1, R = 2-naphthyl, R2R3 = OCH:CH, ZZ1 = piperidine-4,1-diyl). Data for biol. activity of I were given.

IT 327173-90-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of heteroannelated pyridines as 5-HT1A receptor ligands)

RN 327173-90-0 CAPLUS  
CN 1H-Indole-5-carboxaldehyde, 3-[2-(4-(1H-pyrrolo[3,2-c]pyridin-4-yl)-1-piperazinyl]ethyl)- (CA INDEX NAME)



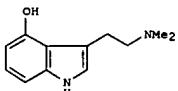
REFERENCE COUNT:  
FORMAT:

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

*R<sup>3</sup> R<sup>4</sup>* X

L10 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2002:19828 CAPLUS  
DOCUMENT NUMBER: 136:263284

TITLE: The chemistry of indoles. Part 109. Synthetic studies of psilocin analogs having either a formyl group or bromine atom at the 5- or 7-position  
AUTHOR(S): Yamada, Fumio; Tamura, Mayumi; Hasegawa, Atsuko; Somei, Masanori  
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Kanazawa University, Kanazawa, 920-0934, Japan  
SOURCE: Chemical & Pharmaceutical Bulletin (2002), 50(1), 92-99  
CODEN: CPBTAL; ISSN: 0009-2363  
PUBLISHER: Pharmaceutical Society of Japan  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 136:263284  
GI

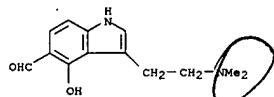


I

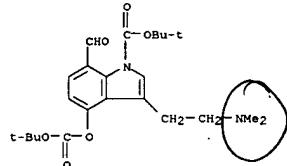
AB Psilocin (I) analogs having either a formyl group or a bromine atom at the 5- or 7-position have been prepared for the first time. Syntheses of 5- and 7-bromo derivs. of 4-hydroxy- and 4-benzyl oxyindole-3-carbaldehyde, 4-benzyl oxyindole-3-acetonitriles, and 4-benzyl oxy-N,N-dimethyltryptamine have also been established.

IT 404887-81-6P 404887-83-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactants or reagent); (synthesis of psilocin analogs having either a formyl group or bromine atom at the 5- or 7-position)

RN 404887-81-6 CAPLUS  
CN 1H-Indole-3-carboxaldehyde, 3-[2-(dimethylamino)ethyl]-4-hydroxy- (CA INDEX NAME)

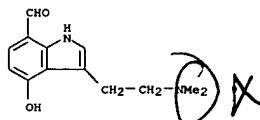


L10 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

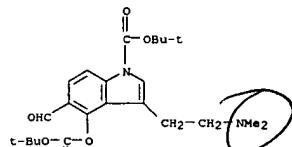


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L10 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
RN 404887-83-8 CAPLUS  
CN 1H-Indole-7-carboxaldehyde, 3-[2-(dimethylamino)ethyl]-4-hydroxy- (CA INDEX NAME)



IT 404887-84-9P 404887-85-0P  
RL: SPN (Synthetic preparation); PREP (Preparation); (synthesis of psilocin analogs having either a formyl group or bromine atom at the 5- or 7-position)  
RN 404887-84-9 CAPLUS  
CN 1H-Indole-1-carboxylic acid, 3-[2-(dimethylamino)ethyl]-4-[(1,1-dimethyl ethoxy)carbonyl]oxy-5-formyl-, 1,1-dimethyl ethyl ester (CA INDEX NAME)



RN 404887-85-0 CAPLUS  
CN 1H-Indole-1-carboxylic acid, 3-[2-(dimethylamino)ethyl]-4-[(1,1-dimethyl ethoxy)carbonyl]oxy-7-formyl-, 1,1-dimethyl ethyl ester (CA INDEX NAME)

L10 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:546477 CAPLUS

DOCUMENT NUMBER: 141:89009

TITLE: Synthesis of tryptamine derivatives and intermediates

thereof

INVENTOR(S): Berens, Ulrich; Dosenbach, Oliver; Sprenger, Daniel

PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.

SOURCE: PCT Int. Appl., 88 pp.

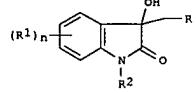
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056769	A2	20040708	WO 2003-EP50992	20031212
WO 2004056769	A3	20040916		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD				
TG: CA 2508290 A1 20040708 CA 2003-2508290 20031212				
AU 2003299227 A1 20040714 AU 2003-299227 20031212				
EP 1572647 A2 20050914 EP 2003-799560 20031212				
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, PL, TX, BG, CZ, SE, HU, SK				
CN 1729174 A 20060201 CN 2003-80107086 20031212				
JP 2006516128 T 20060622 JP 2004-561492 20031212				
US 2006058367 A1 20060316 US 2005-539151 20050616				
IN 2005CN01638 A 20070622 EP 2002-406128 A 20021220				
PRIORITY APPLN. INFO.:				
WO 2003-EP50992 W 20031212				

OTHER SOURCE(S): MARPAT 141:89009  
GI

Instant

L10 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

AB: Indoleacetates I (R = CO2R3; R1 = (un)substituted alkyl, aryl, heterocyclyl, alkylsulfonyl, OH, SH, NO2, halogen, CN, CONH2, CONHNH2, CO2H, alkenyl, alkynyl, cycloalkyl, acyloxy, NH2, NHNNH2, B(OH)2; R2 = H, (un)substituted alkyl, CO2H, arylsulfonyl, alkylsulfonyl, aryl, CONH2, silyl; R3 = (un)substituted alkyl; n = 0-4) were prepared and converted to I

(R = CONR4R5; R4, R5 = (un)substituted alkyl; R4R5 = (un)substituted alkylene) which were in turn converted to indoleacetamides and tryptamines. The synthesis methods and products are useful in the synthesis of pharmaceuticals. Thus, 5-bromoindolin was treated with CH2(CO2H)2 and ClCONMe2 to give I (R = CONMe2, R1 = 5-Br, R2 = H) which was treated with BF3.Et2O and BH3.Me2SO to give

2-(5-bromo-1H-indol-3-yl)-

N,N-dimethylacetamide or with BF3.Et2O and NaBH4 to give

[2-(5-bromo-1H-indol-3-yl)ethyl]-N,N-dimethylacetamide.

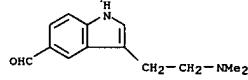
IT: 152673-51-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tryptamine derivs. and intermediates thereof)

RN: 152673-51-3 CAPLUS

CN: 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



L10 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:811739 CAPLUS

DOCUMENT NUMBER: 143:229863

TITLE: A manufacturing of (triazolylmethyl)indole

derivatives

and their intermediates

INVENTOR(S): Martin, Pierre; Berens, Ulrich; Boudier, Andreas;

Dosenbach, Oliver

PATENT ASSIGNEE(S): Ratiopharm G.m.b.H., Germany

SOURCE: PCT Int. Appl. 67 pp.

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

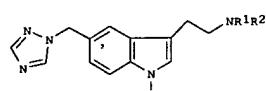
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005075422	A1	20050818	WO 2005-EP793	20050127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, T2, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2553652	A1	20050818	CA 2005-2553652	20050127
EP 1751104	A1	20070214	EP 2005-707035	20050127
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
IN 2006DN03983	A	20070824	IN 2006-DN3983	20060711
US 2007123711	A1	20070531	US 2006-586958	20061128
PRIORITY APPLN. INFO.:				
			US 2004-543463P	F 20040210
			WO 2005-EP793	W 20050127

OTHER SOURCE(S): MARPAT 143:229863

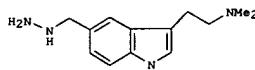
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L10 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

(Continued)



I



II

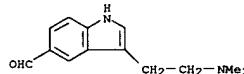
AB The invention relates to a preparation of (triazolylmethyl)indole derivs. of formula I [wherein: R1 and R2 are independently H or alkyl] and their intermediates. For instance, anti-migraine agent rizatriptan I [R1 = R2 = Me; no biol. data] was prepared from [(hydrazinomethylindolyl)ethyl]-dimethyl-amino II with a yield of 55%.

IT 152673-51-3P 862703-18-2P 862703-19-3P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (manufacturing of (triazolylmethyl)indole derivs. and their intermediates)

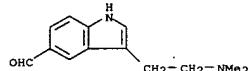
RN 152673-51-3 CAPLUS

CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



RN 862703-18-2 CAPLUS  
CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

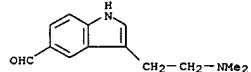
L10 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



● HCl

RN 862703-19-3 CAPLUS  
CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

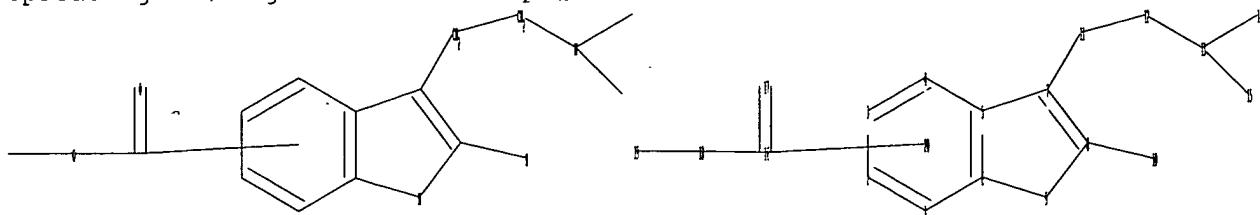
CRN 152673-51-3  
CMF C13 H16 N2 O

CM 2

CRN 144-62-7  
CMF C2 H2 O4

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>  
Uploading C:\Program Files\Stnexp\Queries\10539151\Jan4.str



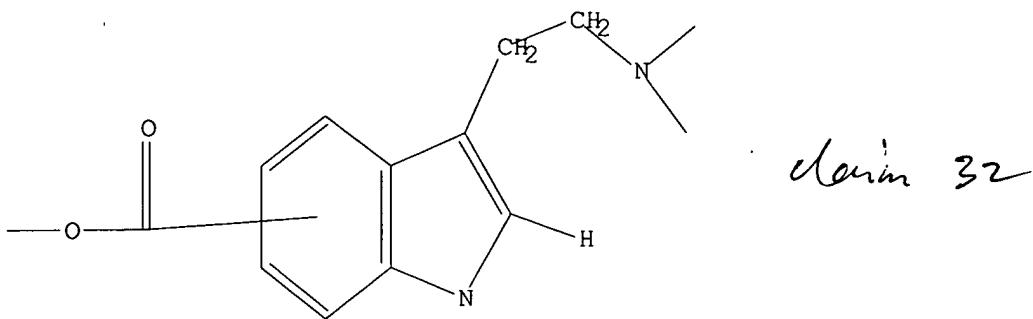
Claim 32

chain nodes :  
10 11 12 16 17 18  
ring nodes :  
1 2 3 4 5 6 7 8 9  
ring/chain nodes :  
13 14 15 19  
chain bonds :  
7-11 8-10 11-12 12-13 16-17 16-18 18-19  
ring/chain bonds :  
13-14 13-15  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9  
exact/norm bonds :  
5-7 6-9 7-8 8-9 13-14 13-15 16-17 16-18 18-19  
exact bonds :  
7-11 8-10 11-12 12-13  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:Atom

L11 STRUCTURE UPLOADED

=> d  
L11 HAS NO ANSWERS  
L11 STR



Structure attributes must be viewed using STN Express query preparation..

=> s l11 full sub=13  
 REG1stRY INITIATED  
 Substance data SEARCH and crossover from CAS REGISTRY in progress...  
 Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 11:38:50 FILE 'REGISTRY'  
 FULL SUBSET SCREEN SEARCH COMPLETED - 5875 TO ITERATE

100.0% PROCESSED 5875 ITERATIONS  
 SEARCH TIME: 00.00.01

7 ANSWERS

L12 7 SEA SUB=L3 SSS FUL L11

SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH  
 L13 6 L12

=> d ibib abs hitstr l13 tot

L13 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2003:234500 CAPLUS

DOCUMENT NUMBER: 139:52822

TITLE: Synthesis of [3-(2-(dimethylamino)ethyl]-2-[{3-(dimethylamino)ethyl}-1H-indol-5-yl]methyl-1H-indol-5-yl]-N-methylmethanesulfonamide - the main sumatriptan impurity

AUTHOR(S): Skwierawska, A.; Palusziewicz, E.

CORPORATE SOURCE: Department of Chemistry, Gdańsk University of Technology, Gdańsk, 80-952, Pol.

SOURCE: Polish Journal of Chemistry (2003), 77(3), 329-332

CODEN: PJCHDQ; ISSN: 0137-5083.

PUBLISHER: Polish Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:52822

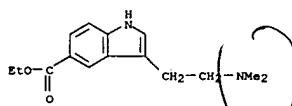
AB Alkylation of sumatriptan in position 2 by 3-(2-(dimethylamino)ethyl)-5-indolemethanol is described. Alternative multistep synthesis of 3-[2-(dimethylamino)ethyl]-5-indolemethanol is presented.

IT 137499-21-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of [3-(2-(dimethylamino)ethyl]-2-[{3-(dimethylamino)ethyl}-1H-indol-5-yl]methyl-1H-indol-5-yl]-N-methylmethanesulfonamide via Fischer indole synthesis)

RN 137499-21-9 CAPLUS

CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester

(CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2001:83714 CAPLUS

DOCUMENT NUMBER: 134:311061

TITLE: Synthesis of 5-(sulfamoylmethyl)indoles  
AUTHOR(S): Bosch, J.; Roca, T.; Armengol, M.; Fernandez-Forner, D.

CORPORATE SOURCE: Laboratory of Organic Chemistry, Faculty of Pharmacy, University of Barcelona, Barcelona, 08028, Spain

SOURCE: Tetrahedron (2001), 57(6), 1041-1048

CODEN: TETRA; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:311061

AB The synthesis of 5-(sulfamoylmethyl)indoles bearing a two-carbon chain at C-3 (aminooethyl, acetate, hydroxyethyl, ethyl) either by the Grandberg modification of the Fischer indolization or by intramol. Heck reaction of suitable o-halotrifluoroacetanilides is reported.

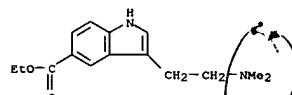
IT 137499-21-9P 334981-33-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of 5-(sulfamoylmethyl)indoles)

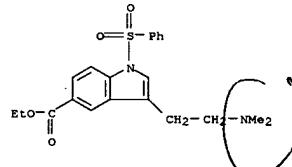
RN 137499-21-9 CAPLUS

CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester

(CA INDEX NAME)



RN 334981-33-8 CAPLUS  
CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-1-(phenylsulfonyl)-, ethyl ester (CA INDEX NAME)



L13 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:610523 CAPLUS

DOCUMENT NUMBER: 123:9441

TITLE: Indole-substituted five-membered heteroaromatic compounds as 5-HT1 receptor agonists

INVENTOR(S): Baker, Raymond; Reeve, Austin J.; Street, Leslie J.

PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK

SOURCE: U.S., 31 pp. Cont. of U.S. Ser. No. 641,422, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

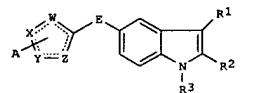
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5317103	A	19940531	US 1992-914683	19920716
PRIORITY APPLN. INFO.:			US 1991-641422	BI 19910115

OTHER SOURCE(S): MARPAT 123:9441

GI



AB The title compds. (I; A = H, halogen, CN, NO2, CF3, (un)substituted NH2, etc.; E = (un)branched Cl-4 alkylene, direct bond; R1 = (un)substituted aminoalkyl, (un)substituted heterocyclyl; R2, R3 = H, Cl-6 alkyl, alkenyl,

alkynyl; W, X, Y, Z = O, S, N, C; Where >1 of W, X, Y, Z = O or S and >1 of W, X, Y, Z = C), useful as specific agonists of 5-HT1-like receptors (no data) and which are useful in the treatment of migraine headache and associated disorders (no data), are prepared and I-containing formulations

presented. Thus, 2-[5-(3-benzyl-1,2,4-oxadiazol-yl)-1H-indol-3-yl]ethylamine hydrogen oxalate hydrate, m.p. 229°, was prepared

IT 137499-21-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of indole-substituted 5-membered heteroaroms. as 5-HT1 receptor agonists)

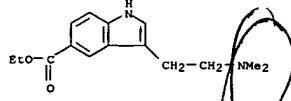
RN 137499-21-9 CAPLUS

CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester

(CA INDEX NAME)



L13 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
 the H<sub>2</sub>oxalate (IV). The activity as agonist of 5-HT<sub>1</sub>-like receptor was measured in terms of their ability to mediate contraction of the sphenous vein of rabbits, and the potency calcd. as -log<sub>10</sub>EC<sub>50</sub> (pEC<sub>50</sub>). The pEC<sub>50</sub> of IV was not less than 5.0. Tablet compns. comprising I are given.  
 IT 137499-21-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, in preparation of 5-HT<sub>1</sub> agonists)  
 RN 137499-21-9 CAPLUS  
 CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester  
 (CA INDEX NAME)

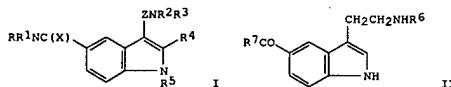


L13 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
 OTHER SOURCE(S): MARPAT 93:132369  
 GI

L13 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
 ACCESSION NUMBER: 1980:532369 CAPLUS  
 DOCUMENT NUMBER: 93:132369  
 ORIGINAL REFERENCE NO.: 93:21105a, 21108a  
 TITLE: Indole compounds and pharmaceutical compositions containing them  
 INVENTOR(S): Webb, Colin Frederick  
 PATENT ASSIGNEE(S): Glaxo Group Ltd., UK  
 SOURCE: Ger. Offen., 102 pp.  
 CODEN: GWKXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2940687	A1	19800430	DE 1979-2940687	19791008
DE 2940687	C2	19910801		
ZA 7905239	A	19801126	ZA 1979-5239	19791002
FI 7903071	A	19800413	FI 1979-3071	19791004
DK 7904255	A	19800413	DK 1979-4255	19791009
AU 7951657	A	19800417	AU 1979-51657	19791010
AU 531783	B2	19830908		
GB 2035310	A	19800618	GB 1979-35208	19791010
GB 2035310	B	19821222		
US 4252803	A	19810224	US 1979-83343	19791010
AT 7906605	A	19840815	AT 1979-6605	19791010
AT 377511	B	19850325		
SE 7908443	A	19800413	SE 1979-8443	19791011
SE 448628	B	19870309		
SE 448628	C	19870618		
CH 646151	A5	19841115	CH 1979-9194	19791011
BE 879381	A1	19800201	BE 1979-197621	19791012
NL 7907583	A	19800415	NL 1979-7583	19791012
FR 2438651	A1	19800509	FR 1979-25446	19791012
FR 2438651	B1	19830304		
JP 55062063	A	19800510	JP 1979-130944	19791012
JP 63058017	B	19881117		
CA 1146550	A1	19830517	CA 1979-337443	19791012
ES 485830	A5	19801030	ES 1979-485830	19791012
PRIORITY APPLN. INFO.:			GB 1978-40279	A 19781012
			JP 1978-138402	A 19781111
			JP 1979-73064	A 19790612

L13 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

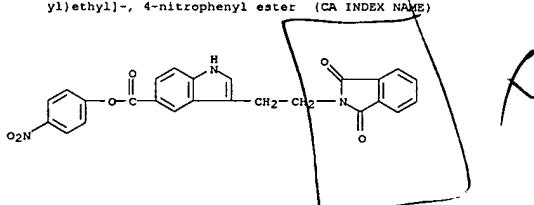


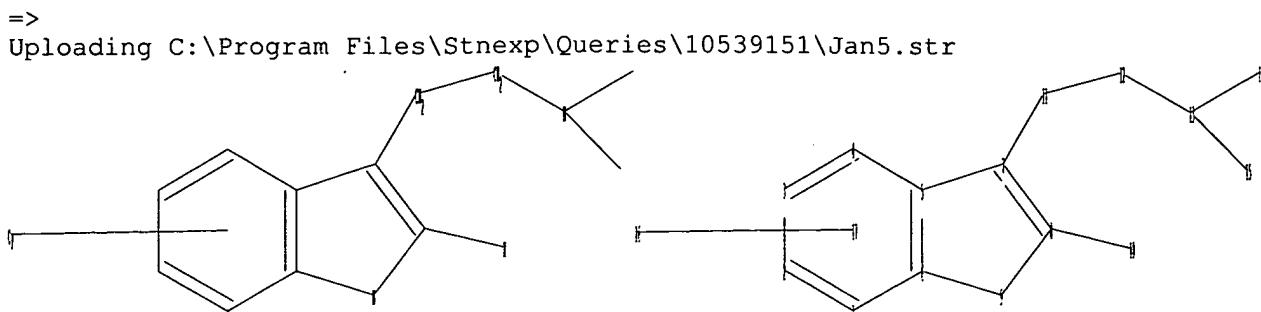
AB The indole derivs. I (R, R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> = H, (substituted) alkyl, cycloalkyl, aryl, or aralkyl; R<sub>1</sub>N, and R<sub>2</sub>R<sub>3</sub>N = ring; R<sub>4</sub> = H, Cl-3 alkyl, aryl; R<sub>5</sub> = H, alkyl, aralkyl; Z = Cl-4 alkylene; X = O, S) and their salts were prepared for use in treatment of hypertension and migraines (no data). Thus, II (R<sub>6</sub> = CO<sub>2</sub>CH<sub>2</sub>Ph, R<sub>7</sub> = OH) reacted with PhCH<sub>2</sub>NH<sub>2</sub> in the presence of

2-chloro-1-methylpyridinium iodide to give II (R<sub>6</sub> = CO<sub>2</sub>CH<sub>2</sub>Ph, R<sub>7</sub> = NHCH<sub>2</sub>Ph), which was hydrogenated over Pd-C to give I (R<sub>6</sub> = H, R<sub>7</sub> = NHCH<sub>2</sub>Ph), isolated as compound with creatinine sulfate.

IT 74884-82-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and amidation of)

RN 74884-82-5 CAPLUS  
 CN 1H-Indole-5-carboxylic acid, 3-[2-(1,3-dihydro-1,3-dioxo-2H-isindol-2-yl)ethyl]-, 4-nitrophenyl ester (CA INDEX NAME)



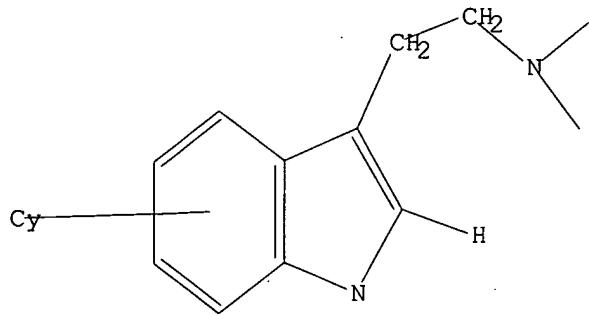


chain nodes :  
 10 11 12 16  
 ring nodes :  
 1 2 3 4 5 6 7 8 9  
 ring/chain nodes :  
 13 14 15  
 chain bonds :  
 7-11 8-10 11-12 12-13  
 ring/chain bonds :  
 13-14 13-15  
 ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9  
 exact/norm bonds :  
 5-7 6-9 7-8 8-9 13-14 13-15  
 exact bonds :  
 7-11 8-10 11-12 12-13  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom  
 Generic attributes :  
 16:  
 Saturation : Unsaturated

L14 STRUCTURE UPLOADED

=> d  
 L14 HAS NO ANSWERS  
 L14 STR



claim 41  
(XIV')

Structure attributes must be viewed using STN Express query preparation.

=> s 114 full sub=13  
REGISTRY INITIATED  
Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 11:42:05 FILE 'REGISTRY'  
FULL SUBSET SCREEN SEARCH COMPLETED - 5875 TO ITERATE

100.0% PROCESSED 5875 ITERATIONS ✓  
SEARCH TIME: 00.00.01

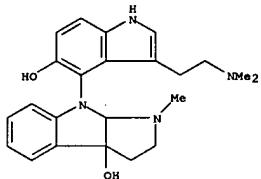
L15 26 SEA SUB=L3 SSS FUL L14

SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH  
L16 11 L15

=> d ibib abs hitstr 116 tot ✓

L16 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:692189 CAPLUS  
 DOCUMENT NUMBER: 142:236417  
 TITLE: Alkaloids from Arundo donax. XVI. Structure of the  
 New  
 AUTHOR(S): Dimeric Indole Alkaloid Arundavine  
 Khuzhaev, V. U.; Zhalolov, I.; Turgunov, K. K.;  
 Tashkodzhaev, B.; Levkovich, M. G.; Aripova, S. F.;  
 Shashkov, A. S.  
 CORPORATE SOURCE: Kokand State Pedagogical Institute, Uzbekistan  
 SOURCE: Chemistry of Natural Compounds (translation of  
 Khimiya  
 Prirodnikh Soedinenii) (2004), 40(3), 261-265  
 CODEN: CHNCAB; ISSN: 0009-3130  
 PUBLISHER: Kluwer Academic/Consultants Bureau  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The new bis-indole alkaloid arundavine, a tryptamine-tryptamine base, was  
 isolated from roots of Arundo donax. The dimer consists of monomeric  
 units of two known indole alkaloids, alline and bufotenine, joined  
 through the N1 and C4' atoms, resp., to give the structure 8-[3-(2-  
 dimethylaminoethyl)-5-hydroxy-1H-indol-4-yl]-1-methyl-2,3,8a-tetrahydro-  
 1H-pyrrolo[2,3-b]indol-3a-ol.  
 IT 844696-24-8, Arundavine  
 RL: BSB (Biological study, unclassified); NPO (Natural product  
 occurrence); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)  
 (structure of new dimeric indole alkaloid arundavine)  
 RN 844696-24-8 CAPLUS  
 CN Pyrrolo[2,3-b]indol-3a(1H)-ol,  
 8-[3-(2-(dimethylamino)ethyl)-5-hydroxy-1H-  
 indol-4-yl]-2,3,8a-tetrahydro-1-methyl- (CA INDEX NAME)

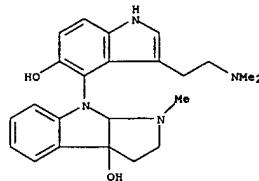
Currently available stereo shown.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

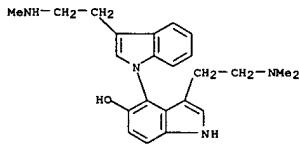
L16 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:541463 CAPLUS  
 DOCUMENT NUMBER: 142:236397  
 TITLE: Alkaloids of the flora of Uzbekistan, Arundo donax  
 AUTHOR(S): Khuzhaev, V. U.  
 CORPORATE SOURCE: S. Yu. Yunusov Institute of the Chemistry of Plant  
 Substances, Tashkent and Kokand State Pedagogic  
 Institute, Academy of Sciences of the Republic of  
 Uzbekistan, Kokand, Uzbekistan  
 SOURCE: Chemistry of Natural Compounds (Translation of  
 Khimiya  
 Prirodnikh Soedinenii) (2004), 40(2), 160-162  
 CODEN: CHNCAB; ISSN: 0009-3130  
 PUBLISHER: Kluwer Academic/Consultants Bureau  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Alkaloids of Arundo donax L. growing in four soil-climatic regions of  
 Uzbekistan were studied. Twenty alkaloids, including the new ones  
 arundavine and arundanine, were isolated from the plant.  
 IT 844696-24-8P, Arundavine  
 RL: NPO (Natural product occurrence); PUR (Purification or recovery);  
 BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (new alkaloids isolated from Arundo donax)  
 RN 844696-24-8 CAPLUS  
 CN Pyrrolo[2,3-b]indol-3a(1H)-ol,  
 8-[3-(2-(dimethylamino)ethyl)-5-hydroxy-1H-  
 indol-4-yl]-2,3,8a-tetrahydro-1-methyl- (CA INDEX NAME)

Currently available stereo shown.

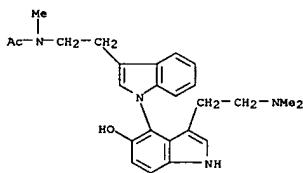


IT 475977-53-8, Arundamine 492994-31-7, Arundacine  
 618852-71-4, Arundanine  
 RL: BSB (Biological study, unclassified); BIOL (Biological study)  
 (of Arundo donax growing in Uzbekistan)  
 RN 475977-53-8 CAPLUS  
 CN [1,4'-Bi-1H-indol]-5'-ol, 3'-(2-(dimethylamino)ethyl)-3-[2-(methylamino)ethyl]- (CA INDEX NAME)

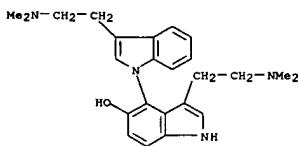
L16 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 492994-31-7 CAPLUS  
 CN Acetamide,  
 N-(2-[3'-(2-(dimethylamino)ethyl)-5'-hydroxy[1,4'-bi-1H-indol]-  
 3-yl]ethyl)-N-methyl- (CA INDEX NAME)

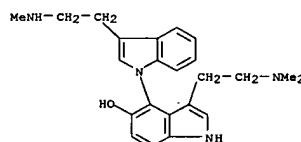


RN 618852-71-4 CAPLUS  
 CN [1,4'-Bi-1H-indol]-5'-ol, 3,3'-bis[2-(dimethylamino)ethyl]- (CA INDEX  
 NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

L16 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:541433 CAPLUS  
 DOCUMENT NUMBER: 142:156195  
 TITLE: Alkaloids from Arundo donax L. X. Mass spectrometric  
 fragmentation of Arundamine and Arundanine  
 AUTHOR(S): Khuzhaev, V. U.  
 CORPORATE SOURCE: S. Yu. Yunusov Institute of the Chemistry of Plant  
 Substances, Academy of Sciences of the Republic of  
 Uzbekistan, Tashkent, Uzbekistan  
 SOURCE: Chemistry of Natural Compounds (Translation of  
 Khimiya  
 Prirodnikh Soedinenii) (2004), 40(2), 196-197  
 CODEN: CHNCAB; ISSN: 0009-3130  
 PUBLISHER: Kluwer Academic/Consultants Bureau  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The mass spectrometric fragmentation of arundamine (1) and arundanine (2)  
 isolated from Arundo donax was studied in light of the structures  
 established for them. The compds. differ in ion mol. weight by 14 amu.  
 Therefore, the fragmentation of these compds. is observed to be  
 completely  
 parallel. Thus, elimination from the side chains of a C2H6N fragment  
 produces strong peaks with m/z 332 (for 1) and 346 (for 2). Loss of a  
 C3H8N fragment (58 amu) in turn leads to ions with m/z 318 (1) and 332  
 (2), resp. Loss of the side chains in both instances gives rise to peaks  
 with m/z of 273 and 259. Elimination of fragments of 28 amu converts  
 them  
 to ions with m/z 245 and 231, resp.  
 IT 475977-53-8, Arundamine 618852-71-4, Arundanine  
 RL: BSB (Biological study, unclassified); PRP (Properties); BIOL  
 (Biological study)  
 (mass spectrometric fragmentation of arundamine and arundanine,  
 alkaloids from Arundo donax)  
 RN 475977-53-8 CAPLUS  
 CN [1,4'-Bi-1H-indol]-5'-ol, 3'-(2-(dimethylamino)ethyl)-3-[2-(methylamino)ethyl]- (CA INDEX NAME)



RN 618852-71-4 CAPLUS  
 CN [1,4'-Bi-1H-indol]-5'-ol, 3,3'-bis[2-(dimethylamino)ethyl]- (CA INDEX  
 NAME)

L16 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

(Continued)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L16 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:566669 CAPLUS

DOCUMENT NUMBER: 139:348106

TITLE: Alkaloids of Arundo donax L. 13. The structure of a new dimeric indole alkaloid, arundanine

AUTHOR(S): Khuzhaev, V. U.; Zhalolov, I. Zh.; Levkovich, M. G.;

CORPORATE SOURCE: Kokand State Pedagogical Institute, Kokand,

SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (2003), 52(3), 745-747

CODEN: RCBUEY; ISSN: 1066-5285

PUBLISHER: Kluwer Academic/Consultants Bureau

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The structure of a new dimeric indole alkaloid, named arundanine (I), isolated from the roots of *Arundo donax* L. (Poaceae), was elucidated. I was identified as 3-(N,N-dimethylaminoethyl)-4-[3-(N,N-dimethylaminoethyl)indole-1-yl]-5-hydroxyindole on the basis of spectroscopic data and the transformation into the known alkaloid, arundamine (II).

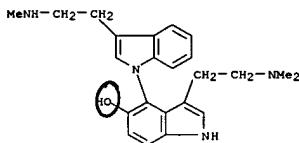
IT 475977-53-8, Arundamine

RL: RCT (Reactant); RACT (Reactant or reagent)

(new dimeric indole alkaloid arundanine of *Arundo donax* transformation to arundamine)

RN 475977-53-8 CAPLUS

CN [1,4'-Bi-1H-indol]-5'-ol, 3'-(2-(dimethylamino)ethyl)-3-[2-(methylamino)ethyl]- (CA INDEX NAME)

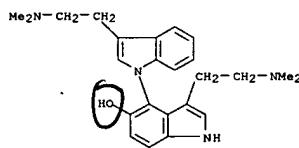


IT 619852-71-4P, Arundanine

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or reagent)

(structure of new dimeric indole alkaloid arundanine of *Arundo donax*)

L16 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 618852-71-4 CAPLUS  
CN [1,4'-Bi-1H-indol]-5'-ol, 3,3'-bis[2-(dimethylamino)ethyl]- (CA INDEX NAME)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L16 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:795021 CAPLUS

DOCUMENT NUMBER: 137:382263

TITLE: Alkaloids of *Arundo donax*. IX. Crystal structure of arundamine

AUTHOR(S): Zhalolov, I. Zh.; Tashkhodzhaev, B.; Khuzhaev, V. U.; Aripova, S. F.

CORPORATE SOURCE: S. Yu. Yunusov Institute of the Chemistry of Plant Substances, Academy of Sciences of the Republic of Uzbekistan, Tashkent, Uzbekistan

SOURCE: Chemistry of Natural Compounds (Translation of

Prirodnnykh Soedinenii) (2002), 38(1), 83-86

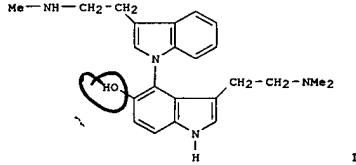
CODEN: CHNCAB; ISSN: 0009-3130

PUBLISHER: Kluwer Academic/Consultants Bureau

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB An x-ray structure anal. was performed for the new dimeric alkaloid arundamine (I) isolated from *Arundo donax*. Its properties are reported.

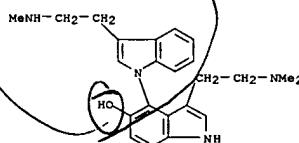
IT 475977-53-8P, Arundamine

RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(crystal structure of arundamine from *Arundo donax*)

RN 475977-53-8 CAPLUS

CN [1,4'-Bi-1H-indol]-5'-ol, 3'-(2-(dimethylamino)ethyl)-3-[2-(methylamino)ethyl]- (CA INDEX NAME)



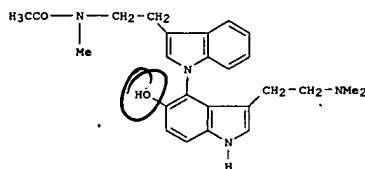
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS

Searched by Jason M. Nolan, Ph.D.

Page 36

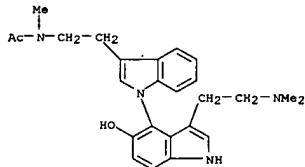
L16 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
RECORD. ALL CITATIONS AVAILABLE IN THE RE  
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L16 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2002:750364 CAPLUS  
DOCUMENT NUMBER: 138:133835  
TITLE: Alkaloids of Arundo donax. XII. Structure of the new dimeric indole alkaloid arundacine  
AUTHOR(S): Khuzhaev, V. U.; Zhalolov, I. Zh.; Levkovich, M. G.; Aripova, S. F.; Shashkov, A. S.  
CORPORATE SOURCE: S. Yu. Yunusov Institute of the Chemistry of Plant Substances, Academy of Sciences of the Republic of Uzbekistan, Tashkent, Uzbekistan  
SOURCE: Khimiya  
PUBLISHER: Prirodnykh Soedinenii (2002), 38(3), 280-283  
DOCUMENT TYPE: CODEN: CHNCA8; ISSN: 0009-3130  
LANGUAGE: Kluwer Academic/Consultants Bureau  
GI: Journal  
English



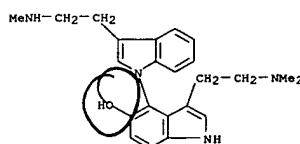
AB The new dimeric indole alkaloid arundacine (I) was isolated from the polar fraction of the total alkaloids from Arundo donax L. roots. The structure 3-N,N-dimethylaminoethyl-5-hydroxy-4-(3'-N'-acetyl-N'-methylaminoethylindol-1'-yl)indole was established using spectral data (IR, UV, mass, one-dimensional <sup>1</sup>H and <sup>13</sup>C NMR, various two-dimensional spectra).  
IT 492994-31-7P, Arundacine  
RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
RN 492994-31-7 CAPLUS  
CN Acetamide,  
N-[2-[3-[(2-(dimethylamino)ethyl)-5'-hydroxy[1,4'-bi-1H-indol-3-yl]ethyl]-N-methyl- (CA INDEX NAME)

L16 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L16 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2002:750363 CAPLUS  
DOCUMENT NUMBER: 138:137449  
TITLE: Alkaloids of Arundo donax. XI. NMR spectroscopic study  
AUTHOR(S): Zhalolov, I. Zh.; Khuzhaev, V. U.; Levkovich, M. G.; Aripova, S. F.; Shashkov, A. S.  
CORPORATE SOURCE: S. Yu. Yunusov Institute of the Chemistry of Plant Substances, Academy of Sciences of the Republic of Uzbekistan, Tashkent, Uzbekistan  
SOURCE: Khimiya  
PUBLISHER: Prirodnykh Soedinenii (2002), 38(3), 276-279  
DOCUMENT TYPE: CODEN: CHNCA8; ISSN: 0009-3130  
LANGUAGE: Kluwer Academic/Consultants Bureau  
Journal  
English  
AB The dimeric indole alkaloid arundamine was isolated from the total bases of Arundo donax L. (Poaceae) roots. The structure of arundamine was investigated using ordinary one-dimensional <sup>1</sup>H and <sup>13</sup>C NMR, J-modulated <sup>13</sup>C NMR, and various types of two-dimensional spectra, COSY, NOESY, HSQC, and HMBC.  
IT 475977-53-8, Arundamine  
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)  
(NMR spectroscopic study of structure of dimeric alkaloid arundamine)  
RN 475977-53-8 CAPLUS  
CN [1,4'-Bi-1H-indol]-5'-ol, 3'-(2-(dimethylamino)ethyl)-3-(2-(methylamino)ethyl)- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L16 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:247954 CAPLUS

DOCUMENT NUMBER: 126:225161

TITLE: Acylated derivatives of melatonin and its analogs, useful as medicaments

INVENTOR(S): Fourtillan, Jean-Bernard; Fourtillan, Marianne; Jacqusey, Jean-Claude; Jouannetaud, Marie-Paule;

Violeau, Bruno; Karam, Omar

PATENT ASSIGNEE(S): Cemaf, Fr.; Laboratoires Besins Iacovesco S.A.; Fourtillan, Jean-Bernard; Fourtillan, Marianne;

Jacqusey, Jean-Claude; Jouannetaud, Marie-Paule;

Violeau, Bruno; Karam, Omar

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

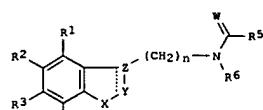
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9706140	A1	19970220	WO 1996-FR1260	19960807
W: AL, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IS, JP, KP, KR, LK, LR, LT, LV, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, TJ, TM				
FR: BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
FR 2737725	A1	19970214	FR 1995-9611	19950808
FR 2737725	B1	19971031		
AU 9668236	A	19970305	AU 1996-68236	19960807
EP 851855	A1	19980708	EP 1996-928490	19960807
EP 851855	B1	20020605		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1196049	A	19981014	CN 1996-196943	19960807
CN 1118451	B	20030820		
JP 11510804	T	19990921	JP 1996-508184	19960807
AT 218547	T	20020615	AT 1996-928490	19960807
PT 851855	T	20021031	PT 1996-928490	19960807
ES 2176480	T3	20021201	ES 1996-928490	19960807
ZA 9606751	A	19971103	ZA 1996-6751	19960808
US 6004991	A	19991221	US 1998-11042	19980327
US 6140372	A	20001031	US 1999-292968	19990416
PRIORITY APPLN. INFO.:			FR 1995-9611	A 19950808
			WO 1996-FR1260	W 19960807

OTHER SOURCE(S): CASREACT 126:225161; MARPAT 126:225161

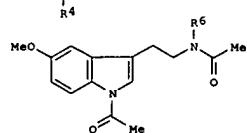
GI

L16 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

(Continued)



I



II

AB Title derivs. I [W = O, S, (un)substituted NH; X = (un)substituted NH, CH:CH, CH2CH2; YZ = CH:C, C(W)CH, CH2CH; or XYZ = (un)substituted CH2CH:CHCH, CH2C(W)CH2CH, CH2CH2C(W)CH; n = 1-4, especially 2; R1-R6 = H, OH, (un)substituted alk(en)ynyl, cycloalkyl, alkoxy, aryloxy, aralkoxy, alkylthio, halo, NO2, aryl, etc.], are disclosed, as is a method for their preparation, their therapeutic use, particularly for treating diseases associated with melatonin disorders, and pharmaceutical and cosmetic compns. containing them. For example, treatment of melatonin with NaH in THF, followed by acetyl chloride, gave title compds. II [R6 = H and Ac]. Tests in fish showed that I have a hypnotic effect greater than that of melatonin, and equivalent to that of diazepam.

IT 188397-12-8P

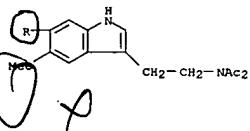
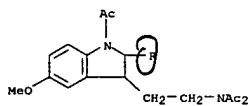
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

RN 188397-12-8 CAPLUS

CN Acetamide, N,N'-{[(1-acetyl-2,3-dihydro-5,5'-dimethoxy[2,6'-bi-1H-indole]-3,3'-diyl)di-2,1-ethanediyl]bis[N-acetyl- (9CI) (CA INDEX NAME)

L16 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

(Continued)



L16 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:774512 CAPLUS

DOCUMENT NUMBER: 123:339506

TITLE: Reaction of malondialdehyde with amine neurotransmitters. Formation and oxidation chemistry of fluorescent dihydropyridines adducts

AUTHOR(S): d'Ischia, Marco; Napolitano, Alessandra; Costantini, Claudio

CORPORATE SOURCE: Department Organic Biological Chemistry, University Naples Federico II, Naples, I-80134, Italy

SOURCE: Tetrahedron (1995), 51(34), 9501-8

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Under physiol. relevant conditions, malondialdehyde reacts smoothly with amine neurotransmitters, i.e. dopamine, norepinephrine and serotonin, to give fluorescent dihydropyridines as the relatively most abundant products. Small ams. of enaminol derivs. could also be obtained in the reactions with dopamine and serotonin. Oxidation of 1-(2-(3,4-dihydroxyphenyl)ethyl)-4-methyl-1,4-dihydro-3,5-pyridinedicarboxaldehyde with hydrogen peroxide/peroxidase leads to a complex pattern of unstable products, the major of which has been isolated and identified as a o-quinone epoxide. Similar oxidation of the other dihydropyridines affords

mainly the N-unsubstituted dihydropyridine and the 4,4'-biindolyl derivative, resp. These results provide new clues to the role of malondialdehyde in neuronal degeneration and lipofuscin formation.

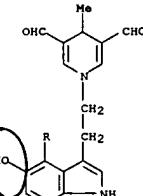
IT 170803-42-6P

RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation) (1,4-dihydropyridine adducts from malondialdehyde and neurotransmitter amines)

RN 170803-42-6 CAPLUS

CN 3,5-Pyridinedicarboxaldehyde, 1,1'-(5,5'-dihydroxy[4,4'-bi-1H-indole]-3,3'-diyl)di-2,1-ethanediyl]bis[1,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)

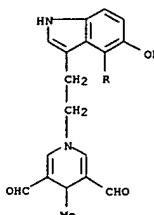
PAGE 1-A



L16 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

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PAGE 2-A



L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

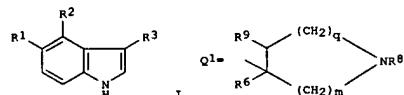
ACCESSION NUMBER: 1995:557092 CAPLUS

DOCUMENT NUMBER: 122:290709

TITLE: Preparation of tryptamine analogs as 5-HT1-like agonists or partial agonists.  
INVENTOR(S): Porter, Roderick Alan; Coates, William John  
PATENT ASSIGNEE(S): SmithKline Beecham PLC, UK  
SOURCE: PCT Int. Appl., 43 pp.  
CODEN: PIXXD2DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9414771	A1	19940707	WO 1993-EP3564	19931214
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9458119	A	19940719	AU 1994-58119	19931214
EP 674620	A1	19951004	EP 1994-903794	19931214
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
JP 08504786	T	19960521	JP 1993-514774	19931214
ZA 9309456	A	19950619	ZA 1993-9456	19931214
CN 1092765	A	19940928	CN 1993-112761	19931220
			GB 1992-26537	A 19921221
PRIORITY APPLN. INFO.:				
			WO 1993-EP3564	W 19931214

OTHER SOURCE(S): MARPAT 122:290709  
GI

AB Title compds. [I; R1 = (substituted) 6-10-membered (hetero)aryl ring; R2 = H, halo, Cl-4 alkyl, CN, NO2, CF3; R3 = CR4R5CH2NR6R7, CH:NNHC(NH)NH2, Q1; R4-R7 = H, Cl-4 alkyl; NR6R7 = ring; R8 = H, Cl-4 alkyl, C3-6 alkenyl; Ra = H; Rb = H, OH; RaRb = bond; q, m = 1, 2], were prepared I are 5-HT1-like agonists or partial agonists and may be useful in the treatment and/or prophylaxis of migraine, cluster headache, headache associated with vascular

L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)  
disorders and other neuralgia. They are also expected to have utility in the treatment or prophylaxis of portal hypertension. Thus, 2-chloro-6-nitro-3-phenyltoluene (prep. given) was heated with DMF di-Me acetal and pyrrolidine in DMF at 120°; the resulting enamine was stirred with N2H4 and Raney Ni in MeOH to give 4-chloro-5-phenylindole. This was stirred with AcCl and bis(dimethylamino)methane in CH2Cl2 to

give a residue which was stirred with KCN and MeI in DMF to give 4-chloro-3-cyanoethyl-5-phenylindole. The latter in MeOH was shaken with Me2NH and Raney Ni under 40 psi H to give 4-chloro-3-[2-(dimethylamino)ethyl]-5-phenylindole. I showed EC50 = 0.03-1.5 μM in the rabbit basilar artery 5-HT1-like receptor screen.

IT 163104-46-9P 163104-47-0P 163104-66-3P  
163104-70-9P 163104-71-0P 163104-85-6P  
163104-86-7P 163104-89-0P 163104-90-3P  
163105-04-2P 163105-07-5P 163105-08-6P  
163105-11-1P 163105-26-8P 163105-27-9P  
163105-29-1P 163105-95-1P

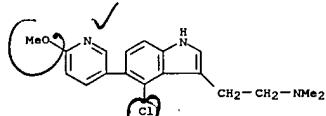
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of tryptamine analogs as 5-HT1-like agonists or partial agonists)

RN 163104-46-9 CAPLUS  
CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-phenyl-

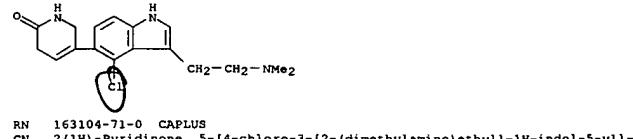
L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

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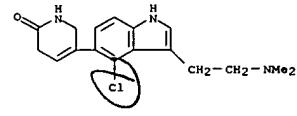
RN 163104-66-3 CAPLUS  
CN 1H-Indole-3-ethanamine, 4-chloro-5-(6-methoxy-3-pyridinyl)-N,N-dimethyl- (CA INDEX NAME)



RN 163104-70-9 CAPLUS  
CN 2(1H)-Pyridinone, 5-(4-chloro-3-[(2-(dimethylamino)ethyl)-1H-indol-5-yl]-3,6-dihydro- (CA INDEX NAME)

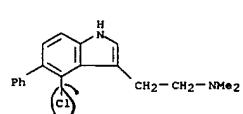


RN 163104-71-0 CAPLUS  
CN 5-(4-chloro-3-[(2-(dimethylamino)ethyl)-1H-indol-5-yl]-3,6-dihydro-, monohydrate (9CI) (CA INDEX NAME)



RN 163104-85-6 CAPLUS  
CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-fluorophenyl)-N,N-dimethyl- (CA INDEX NAME)

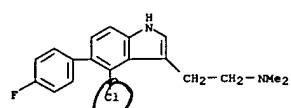
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CRN 163104-46-9  
CMF C18 H19 Cl N2



CM 2

L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

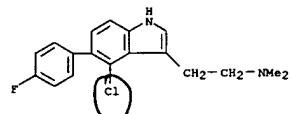
(Continued)



RN 163104-86-7 CAPLUS  
 CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-fluorophenyl)-N,N-dimethyl-ethanedicarboxylate (9CI) (CA INDEX NAME)

CM 1

CRN 163104-85-6  
 CMF C18 H18 Cl F N2

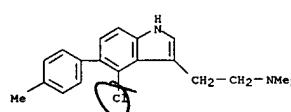


CM 2

CRN 144-62-7  
 CMF C2 H2 O4

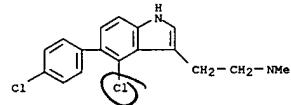


RN 163104-89-0 CAPLUS  
 CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-(4-methylphenyl)- (CA INDEX NAME)



L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

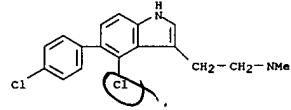
(Continued)



RN 163105-08-6 CAPLUS  
 CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-chlorophenyl)-N,N-dimethyl-ethanedicarboxylate (9CI) (CA INDEX NAME)

CM 1

CRN 163105-07-5  
 CMF C18 H18 Cl2 N2

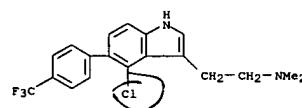


CM 2

CRN 144-62-7  
 CMF C2 H2 O4



RN 163105-11-1 CAPLUS  
 CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 163105-26-8 CAPLUS  
 CN 1H-Indole-3-ethanamine, 4-chloro-5-(2-methoxy-3-pyridinyl)-N,N-dimethyl- (CA INDEX NAME)

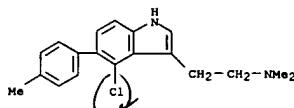
L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

(Continued)

RN 163104-90-3 CAPLUS  
 CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-(4-methylphenyl)-ethanedicarboxylate (9CI) (CA INDEX NAME)

CM 1

CRN 163104-89-0  
 CMF C19 H21 Cl N2

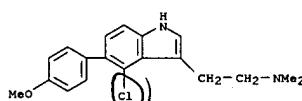


CM 2

CRN 144-62-7  
 CMF C2 H2 O4



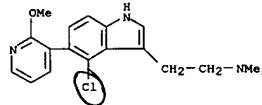
RN 163105-04-2 CAPLUS  
 CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-methoxyphenyl)-N,N-dimethyl- (CA INDEX NAME)



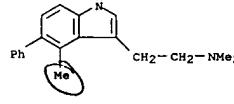
RN 163105-07-5 CAPLUS  
 CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-chlorophenyl)-N,N-dimethyl- (CA INDEX NAME)

L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

(Continued)



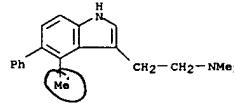
RN 163105-27-9 CAPLUS  
 CN 1H-Indole-3-ethanamine, N,N,4-trimethyl-5-phenyl- (CA INDEX NAME)



RN 163105-29-1 CAPLUS  
 CN 1H-Indole-3-ethanamine, N,N,4-trimethyl-5-phenyl-, ethanedicarboxylate (9CI) (CA INDEX NAME)

CM 1

CRN 163105-27-9  
 CMF C19 H22 N2



CM 2

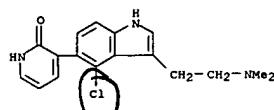
CRN 144-62-7  
 CMF C2 H2 O4



RN 163105-95-1 CAPLUS  
 CN 1H-Pyridinone, 3-[4-chloro-3-(2-(dimethylamino)ethyl)-1H-indol-5-yl]- (CA INDEX NAME)

L16 ANSWER 10 OF 11 CAPLUS' COPYRIGHT 2008 ACS on STN

(Continued)



IT 163105-78-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of tryptamine analogs as 5-HT1-like agonists or partial agonists)

RN 163105-78-0 CAPLUS

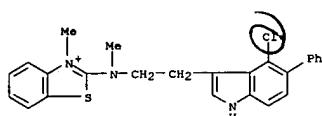
CN Benzothiazolium,

2-[(2-(4-chloro-5-phenyl-1H-indol-3-yl)ethyl)methylamino]-3-methyl-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 163105-77-9

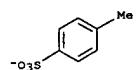
CNF C25 H23 Cl N3 S



CM 2

CRN 16722-51-3

CNF C7 H7 O3 S



L16 ANSWER 11 OF 11 CAPLUS' COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1979:187197 CAPLUS

DOCUMENT NUMBER: 90:187197

ORIGINAL REFERENCE NO.: 90:29756h,29757a

TITLE: Quadrigemines-A and -B, two minor alkaloids of Hodgkinsonia frutescens F. Muell

AUTHOR(S): Perry, Keith P.; Smith, George F.  
CORPORATE SOURCE: Dep. Chem., Univ. Manchester, Manchester, UK  
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1978), (12), 1671-82

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The structures of quadrigemines A (an approx. 1:1 mixture of diastereoisomer I and one (or a mixture of both) of the meso diastereoisomers) and B (II), isolated from *H. frutescens* leaves, were determined by spectroscopic and chemical means. These are the 1st examples of alkaloid structures made up of 4 tryptamine units.IT 69937-12-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 69937-12-8 CAPLUS  
CN [3,7'-Bi-1H-indole]-3,3'-(2H)-diethanamine, N,N,N',N'-tetramethyl-5,5'-dinitro- (9CI) (CA INDEX NAME)